

The integro-moment method applied to two-dimensional rarefied gas flows

S. Varoutis⁽¹⁾, D. Valougeorgis⁽¹⁾ and F. Sharipov⁽²⁾

⁽¹⁾*Department of Mechanical and Industrial Engineering
University of Thessaly
Pedion Areos, Volos, 38333, Greece*

⁽²⁾*Departamento de Fisica
Universidade Federal do Parana
Caixa Postal 19044, Curitiba, 81531-990, Brazil*

Abstract. The integro-moment method (IMM) has been formulated in a simple and concise manner to solve the two-dimensional flow of a single gas in a rectangular duct, described by the linearized BGK equation. Based on this prototype problem, a detailed computational investigation of the IMM with regard to convergence speed, accuracy, storage and CPU time is performed. Overall, it is demonstrated that the IMM may be considered as a reliable alternative computational approach for solving linear multidimensional rarefied gas flows. The IMM is particularly suitable, when the discretization in the molecular velocity space must be avoided in order to eliminate the oscillatory behavior of the computed macroscopic quantities due to the propagation of boundary induced discontinuities.

Keywords: Vacuum flows, Nano and microflows, Non-equilibrium flows, Kinetic theory

PACS: 05.20Dd, 47.45-n, 47.45.Ab, 51.10+y

1. INTRODUCTION

During the last decade there is an increased interest in rarefied gas flows due to their engineering applications in several fields including vacuum systems. The most commonly used computational methods to solve rarefied flows are probabilistic approaches based on the DSMC method and deterministic schemes based on the discrete ordinates or velocity method, which from now on we will denote it by DVM. Although, both techniques have been implemented in a sophisticated manner to solve complex flow configurations, there are still several pitfalls related to their computational efficiency and accuracy. For example, the DSMC method suffers from statistical noise when the flow is slow, while the DVM, which is particular suitable for this type of flows, in several occasions produces an unphysical oscillatory behavior in the macroscopic quantities due to the propagation of boundary induced discontinuities inside the computational domain (ray effects).

An alternative deterministic computational scheme for handling linear (slow) flows is the integro-moment method (IMM). Basic information regarding the formulation of the method and its characteristics are reviewed in [1] and more recently in [2]. The basic advantage of the IMM is that the derived equations are discretized only in the spatial independent variables. Over the years, the IMM has been implemented in a limited number of problems [3, 4, 5], while very recently it has been applied to solve the unsteady behavior of a gas over a plate in harmonic oscillatory motion [6]. However, in all cases considered so far, the flow is one-dimensional.

In the present work, first the IMM is properly formulated to tackle multidimensional problems. The proposed formulation is applied to solve the two-dimensional flow of a single gas in a rectangular duct, described by the linearized BGK equation. It turns out that, the extension of the IMM in multi-dimensional flow configurations, although in principal may look straightforward, it is not trivial. Based on this prototype problem, a detailed

computational investigation of the IMM with regard to convergence speed, accuracy, storage and CPU time is performed. In addition, certain computational and programming issues are resolved in an efficient manner in order the method to be considered as a reliable alternative computational scheme for solving linear multidimensional flows.

2. FORMULATION

The formulation of the IMM is presented by solving the two-dimensional flow of a single gas in a rectangular duct due to pressure gradient. This problem has been solved in [7, 8], by implementing the DVM. Therefore, it is used here as a prototype problem for applying the IMM in two-dimensional flows.

The cross section of the duct is $H \times W$, with H and W denoting the height and the width of the duct respectively. By taking the height H as the characteristic macroscopic length of the problem, the flow domain Ω is defined by $x \in \left[-\frac{W}{2H}, \frac{W}{2H}\right]$ and $y \in \left[-\frac{1}{2}, \frac{1}{2}\right]$ and it is shown in Figure 1. The flow is considered as fully developed in the z direction and end effects in that direction may be neglected. Since the flow is considered as isothermal, the linearized BGK kinetic model can be applied, which for this problem is written as

$$\zeta_x \frac{\partial Y}{\partial x} + \zeta_y \frac{\partial Y}{\partial y} + \delta Y(x, y, \zeta_x, \zeta_y) = \delta u(x, y) - \frac{1}{2}. \quad (1)$$

The unknown distribution function Y has been reduced from the linearized distribution function, following the typical projection procedure in order to eliminate the z component of the molecular velocity vector, which now consists of only two components, i.e. $\zeta = (\zeta_x, \zeta_y)$. The rarefaction parameter δ is proportional to the inverse Knudsen number and it is defined by

$$\delta = \frac{PH}{\mu v_m}, \quad (2)$$

where μ is the shear viscosity, v_m is the most probable molecular velocity, while $u(x, y)$ is the only nonzero component of the macroscopic velocity and it is in the z direction. Applying Maxwell scattering boundary conditions with purely diffuse reflection we find that the outgoing distributions at the boundaries become

$$Y_b^+ = 0. \quad (3)$$

Equation (1) is written in the more convenient form

$$-\zeta \frac{\partial Y}{\partial s} + \delta Y = \delta u - \frac{1}{2}, \quad (4)$$

where the new independent variable s denotes the characteristic direction along the molecular velocity ζ , $\zeta = (\zeta, \varphi)$, with $\zeta_x = \zeta \cos \varphi$ and $\zeta_y = \zeta \sin \varphi$ and

$$u(x, y) = \frac{1}{\pi} \int_0^{2\pi} \int_0^\infty Y e^{-\zeta^2} \zeta d\zeta d\varphi. \quad (5)$$

Multiplying Eq. (1) by $\exp(-\delta s/\zeta)$ and integrating the resulting equation along the characteristic, while ζ is treated as a parameter, we obtain

$$Y(x, y, \zeta, \varphi) = \frac{\delta}{\zeta} \int_0^{s_0} u(x', y') e^{-\delta s / \zeta} ds + \frac{1}{2\delta} (e^{-\delta s_0 / \zeta} - 1). \quad (6)$$

To find Eq. (6) we have also used the boundary condition (3). Substituting Eq. (6) into Eq. (5) and after some routine manipulation we find the following integral equation for the macroscopic velocity:

$$u(x, y) = \frac{\delta}{\pi} \int_0^{2\pi} \int_0^{s_0} T_0(\delta s) u(x', y') ds d\varphi + \frac{1}{2\pi\delta} \int_0^{2\pi} T_1(\delta s_0) d\varphi - \frac{1}{2\delta} \quad (7)$$

As it is shown in Figure 1, s_0 is the distance from a point (x, y) up to the boundary along the characteristic line in the opposite direction of the molecular velocity ζ , the pairs (x', y') denote points along the integration path $s \in [0, s_0]$, with $x' = x - s \cos \varphi$ and $y' = y - s \sin \varphi$, while

$$T_n(\omega) = \int_0^\infty \zeta^n \exp\left(-\zeta^2 - \frac{\omega}{\zeta}\right) d\zeta \quad (8)$$

are the well known Abramowitz functions of order n [9].

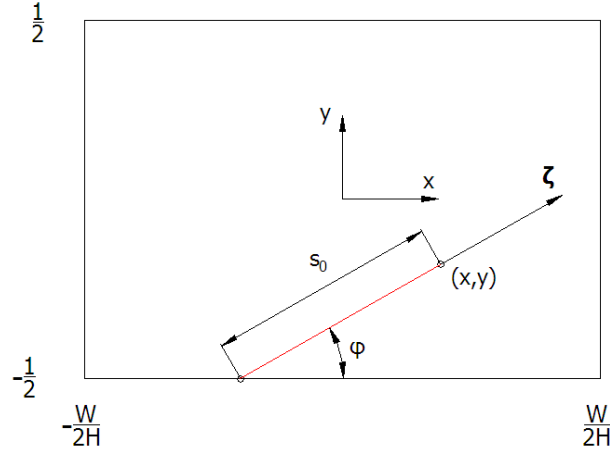


FIGURE 1. The flow domain

Equation (7) is solved numerically in an iterative manner to yield the unknown macroscopic velocity. Another macroscopic quantity of practical interest, which can be readily obtained once the velocity field is known, is the shear stress tensor defined by the vector equation

$$\begin{pmatrix} \Pi_{xz}(x, y) \\ \Pi_{yz}(x, y) \end{pmatrix} = \frac{\delta}{\pi} \int_0^{2\pi} \int_0^{s_0} T_1(\delta s) u(x', y') \begin{pmatrix} \cos \varphi \\ \sin \varphi \end{pmatrix} ds d\varphi + \frac{1}{2\pi\delta} \int_0^{2\pi} T_2(\delta s_0) \begin{pmatrix} \cos \varphi \\ \sin \varphi \end{pmatrix} d\varphi. \quad (9)$$

Also, the non-dimensional flow rate is given by the double integral

$$G = -2 \frac{H}{W} \int_{-\frac{W}{2H}}^{\frac{W}{2H}} \int_{-\frac{1}{2}}^{\frac{1}{2}} u(x, y) dx dy. \quad (10)$$

Before we close this section it is interesting to note that at the free molecular limit, i.e. $\delta \rightarrow 0$, the first term at the right hand side of Eq. (12) vanishes and then, by expanding the $T_1(\omega)$ for $\omega \rightarrow 0$ we deduce the simplified expression

$$\lim_{\delta \rightarrow 0} u(x, y) = \frac{1}{4\sqrt{\pi}} \int_0^{2\pi} s_0 d\varphi, \quad (11)$$

which after it is substituted in Eq. (16) can be integrated analytically to obtain a closed form expression for the flow rate [7].

3. THE NUMERICAL SCHEME

The two-dimensional flow domain is divided in rectangular elements denoted by $(i \times j)$, with $i = 1, \dots, I$ and $j = 1, \dots, J$. The geometrical center of its element is determined by $x_i = (i - 1/2)\Delta x$ and $y_j = (j - 1/2)\Delta y$, where $\Delta x = 1/(A \times I)$ and $\Delta y = 1/J$, while $A = H/W$ is the aspect ratio. The numerical grid is shown in Figure 2.

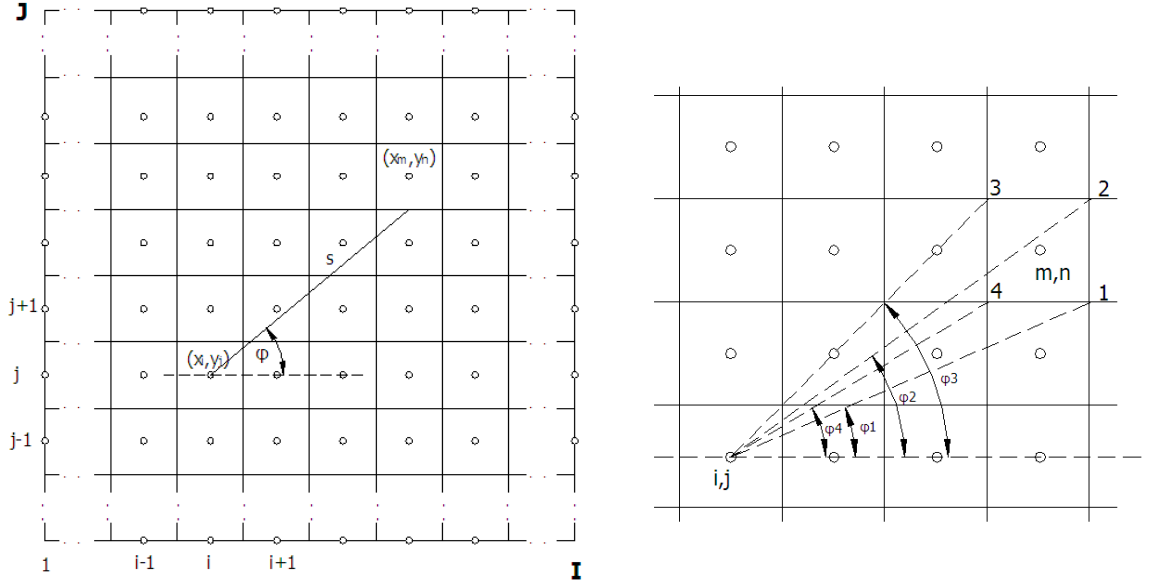


FIGURE 2. The computational grid

Equation (7) is written in the form

$$u(x, y) = \int_{-1/2}^{1/2} \int_{-W/2H}^{W/2H} K(x, y : x', y') u(x', y') dx' dy' + Q(x, y) \quad (12)$$

and then by assuming that the unknown velocities remain constant at each grid element, it may be approximated as

$$u_{ij} = \sum_{m=1}^I \sum_{n=1}^J K_{ij}^{mn} u_{mn} + Q_{ij}, \quad i = 1, \dots, I \quad \text{and} \quad j = 1, \dots, J, \quad (13)$$

where

$$K_{ij}^{mn} = \int_{y_n - \Delta y / 2}^{y_n + \Delta y / 2} \int_{x_m - \Delta x / 2}^{x_m + \Delta x / 2} K(x_i, y_j : x', y') dx' dy'. \quad (14)$$

and

$$Q_{ij} = \frac{1}{2\delta} \left[\frac{1}{\pi} \int_0^{2\pi} T_1(\delta s_0) d\varphi - 1 \right]. \quad (15)$$

The double integrals (14) over a rectangular element can be reduced into single integrals if the variables s and φ , instead of x' and y' , are used. As it is seen in Figure 2, the integration variable s denotes the distance between the node (x_i, y_j) and the sides of the cell (x_m, y_n) , while φ is the corresponding angle with respect to the x axis.

Following this procedure the integration with respect to s becomes analytically and we have to integrate numerically only with respect to φ . In particular, when $i \neq m$ and $j \neq n$ we find

$$K_{ij}^{mn} = -\frac{1}{\pi} \left\{ \int_{\varphi_1}^{\varphi_2} T_1(\delta s_1) d\varphi + \int_{\varphi_2}^{\varphi_3} T_1(\delta s_2) d\varphi + \int_{\varphi_3}^{\varphi_4} T_1(\delta s_3) d\varphi + \int_{\varphi_4}^{\varphi_1} T_1(\delta s_4) d\varphi \right\}, \quad (16)$$

where the distances and the angles are estimated by using typical trigonometric arguments and their values are:

$$s_1 = \frac{x_i - x_n - \Delta x / 2}{\cos \varphi}, \quad s_2 = \frac{y_i - y_m - \Delta y / 2}{\sin \varphi}, \quad s_3 = \frac{x_i - x_n + \Delta x / 2}{\cos \varphi}, \quad s_4 = \frac{y_i - y_m + \Delta y / 2}{\sin \varphi} \quad (17)$$

and

$$\begin{aligned} \varphi_1 &= \tan^{-1} \frac{y_j - y_m + \Delta y / 2}{x_i - x_n - \Delta x / 2}, & \varphi_2 &= \tan^{-1} \frac{y_j - y_m - \Delta y / 2}{x_i - x_n - \Delta x / 2}, \\ \varphi_3 &= \tan^{-1} \frac{y_j - y_m - \Delta y / 2}{x_i - x_n + \Delta x / 2}, & \varphi_4 &= \tan^{-1} \frac{y_j - y_m + \Delta y / 2}{x_i - x_n + \Delta x / 2} \end{aligned} \quad (18)$$

The four angles in (18) are shown in the detail of Figure 2. For the specific case of $i = m$ and $j = n$ the above result is reduced to

$$K_{ij}^{ij} = 1 - \frac{8}{\pi} \int_0^{\pi/4} \left[T_1 \left(\delta \frac{\Delta x / 2}{\cos \varphi} \right) \right] d\varphi. \quad (19)$$

The estimation of all remaining integrals including the one in the source term (15) may be performed numerically by using Newton Cotes formulas. We have found that the application of the trapezoidal rule is adequate to provide results of good accuracy. Once all integrals are computed Eq. (18) is reduced to an algebraic system, which is solved by implementing typical iteration schemes and then the unknowns u_{ij} , with $i = 1, \dots, I$ and $j = 1, \dots, J$ are estimated.

4. REMARKS ON THE COMPUTATIONAL EFFICIENCY OF THE IMM

Following the IMM procedure that we have described in detail in Sections 2 and 3, the flow problem of a single gas through a rectangular duct has been solved for an aspect ratio $A = 1, 0.5$ and 0.1 . In all flow configurations we have used $\Delta x = \Delta y$, with $J = 20, 50$ and 100 , while $I = J / A$. The results, in addition to the velocity field, include

the shear stress tensor and the overall quantities of the flow rate and the drag coefficient at the walls. The accuracy of the results has been tested in several ways. For $\delta = 0$ and $\delta \rightarrow \infty$, analytical results are available, while for the intermediate values of δ the results have been compared with the existing corresponding results based on the DVM [7, 8]. Finally, another way to judge the accuracy to expect from the method is by estimating the drag coefficient, which is constant and independent of δ .

Since, this flow problem has been solved before and all flow quantities of practical interest have been published we choose not to tabulate the results of the present work, which are based on the IMM. Instead, we prefer to proceed with some qualitative and quantitative remarks regarding the computational characteristics of the IMM as well as its plus and minus compared to the DVM.

It has been found that the IMM converges for all values of δ . The speed of convergence is fast for $\delta \leq 0.1$, it slows down as δ is increased and becomes very slow for $\delta \geq 20$. The number of iterations required for convergence is of the same order with the corresponding iterations required in the DVM. A theoretical stability analysis may be applied in future work, at least for simple kinetic models such as the BGK, to confirm these experimental findings.

The required CPU time per iteration in the IMM is proportional to N^2 , where $N = I \times J$ is the total number of nodes, while the corresponding CPU time in the DVM is proportional to $N \times K$, where K is the number of discrete molecular velocities. Therefore, for the present problem, as long as the number of nodes in the physical space is less than in the number of discrete velocities in the molecular velocity space ($N < K$), the IMM runs faster than the DVM and the vice versa when $N > K$. In general, the required CPU time per iteration in the IMM is proportional to N^D , where N is the total number of nodes in the computational domain and D is the number of physical dimensions in the problem.

Regarding accuracy and storage demands we may say that at this stage the DVM performs better. However, the IMM approach may be further improved, while the DVM approach, over the years, has been computational optimized. Probably, a more sophisticated numerical scheme, keeping the simplicity of the one proposed in Section 3 and upgrading at the same time its accuracy may be appropriate.

The most important advantage of the IMM compared to the DVM is that discretization is performed only in the physical space. This is of particular importance in problems with discontinuities in the boundary or the initial conditions. Then, in the DVM these discontinuities are propagating in the computational domain and yield results with an unphysical oscillatory behavior. This pitfall is completely eliminated in the IMM.

Overall, we have found that the IMM is a reliable computational tool for solving this prototype two-dimensional problem. Based on this experience we expect a similar behavior in other more complex multidimensional flows as well.

ACKNOWLEDGMENTS

The work of two of the authors (S.V. and D.V) has been partially funded by the Association EURATOM – Hellenic Republic. This support is gratefully acknowledged. Also, the third author (F. Sh.) thanks CNPq (Brazil) for the support of his research.

REFERENCES

1. M. N. Kogan, *Rarefied gas Dynamics*, Pergamon Press, Oxford, 1969.
2. F. Sharipov and V. Seleznev, Data on internal gas flows, *J. Phys. Chem. Ref. Data*, 27, 657-706, 1998.
3. C. Cercignani and C. D. Pagani, *Phys. Fluids*, 9, 1167, 1966.
4. V. G. Chernyak, B. T. Porodnov and P. E. Suetin, *Zh. Tekhn. Fiz.*, 43, 2420, 1973.
5. P. E. Suetin and V. G. Chernyak, *Izv. Akad. Nauk SSSR. Mekh. Zhidkosti Gaza* N6, 107, 1977.
6. F. Sharipov and D. Kalempa, Gas flow near a plate oscillating longitudinally with an arbitrary frequency, submitted.
7. F. Sharipov, Rarefied gas flow through a long rectangular duct, *J. Vac. Sci. Technol. A*, 3062-3066, 1999.
8. D. Valougeorgis and S. Naris, Acceleration schemes of the discrete velocity method: Gaseous flows in rectangular microchannels", *SIAM J. Sci. Comp.*, 25, 534-552, 2003.
9. M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*. 9th ed., New York: Dover, page 890, 1972.